Finite-Size Scaling of Classical Long-Ranged Ising Chains and the Criticality of Dissipative Quantum Impurity Models

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Motivated in part by quantum criticality in dissipative Kondo systems, we revisit the finite-size scaling of a classical Ising chain with $1/r^{2-\epsilon}$ interactions. For $\frac{1}{2} < \epsilon < 1$, the scaling of the dynamical spin susceptibility is sensitive to the degree of "winding" of the interaction under periodic boundary conditions. Infinite winding yields the expected mean-field behavior, whereas without any winding the scaling is of an interacting ω/T form. The contrast with the behavior of the Bose-Fermi Kondo model suggests a breakdown of a mapping from the quantum model to a classical one due to the smearing of the Kondo spin flips by the continuum limit taken in this mapping.

Quantum criticality describes the collective fluctuations of a continuous quantum phase transition. The standard theoretical picture [1] is that quantum critical fluctuations in d spatial dimensions can be described in terms of the fluctuations of an order parameter (a classical variable) in $d + z$ dimensions, where z is the dynamic exponent. However, there has been much recent interest in quantum critical points (QCPs) that do not conform to this quantum-to-classical mapping [2].

One setting to explore this issue is quantum impurity models that involve one or more dissipative bosonic baths having a sub-ohmic ($\epsilon > 0$) power-law spectrum

$$\sum_p [\delta(\omega - w_p) - \delta(\omega + w_p)] \sim |\omega|^{1-\epsilon} \text{sgn}(\omega) \Theta(\omega_c - |\omega|). \quad (1)$$

Here w_p is the dispersion of the bosonic bath(s) and Θ is the Heaviside function specifying the high-energy cut-off ω_c. The quantum-to-classical mapping leads to a classical Ising chain with $1/r^{2-\epsilon}$ interactions, which has as its continuum limit a local ϕ^4 theory in $0 + 1$ dimension [3]. For $1/2 < \epsilon < 1$, the ϕ^4 theory has a Gaussian fixed point with a violation of ω/T scaling. However, the QCP in a large-N, fixed-κ limit of a spin-rotation-invariant SU(N)×SU(κN) Bose-Fermi Kondo model (BFKM) satisfies ω/T scaling and, hence, is interacting [4]. Numerical renormalization-group (NRG) studies have also found interacting QCPs for $1/2 < \epsilon < 1$ in two quantum models with Ising anisotropy: the dissipative spin-boson model [5] and the Ising BFKM [6]. The failure of the quantum-to-classical mapping has been attributed in the spin-rotation-invariant case to the Berry phase [7], but remains to be clarified for Ising symmetry.

This Letter reports a two-pronged study of the classical mapping of the quantum-critical Ising BFKM. First, we show that, for $1/2 < \epsilon < 1$, the scaling of the dynamical spin susceptibility of the classical model as a function of system size and wave vector (corresponding in the quantum problem to temperature and Matsubara frequency, respectively) depends crucially on the "wind-ing" of the interaction to extend the range of the interaction beyond the finite system size. For infinite winding, one recovers the mean-field $\omega/T^{1/(2-2\epsilon)}$ scaling expected from the corresponding ϕ^4 theory, in which the quartic coupling acts as a dangerously irrelevant variable. Limiting the winding introduces an additional temperature dependence dominating that from the dangerously irrelevant coupling and giving rise for zero winding to ω/T scaling. Second, we provide strengthened evidence for non-mean-field behavior in the BFKM. These findings can be reconciled through a breakdown of the quantum-to-classical mapping arising from failure of the continuum limit to fully preserve the effects of Kondo spin flips.

Bose-Fermi Kondo model and the classical Ising chain.—The BFKM describes a quantum spin coupled to both a fermionic band and a bosonic bath. The Hamiltonian for the Ising-anisotropic case is

$$\mathcal{H}_{\text{BFKM}} = J_K \mathbf{S} \cdot \mathbf{s}_c + \sum_{p\sigma} E_p c^\dagger_{p\sigma} c_{p\sigma}$$
$$+ g S^z \sum_p \left(\phi_p + \phi^\dagger_{-p} \right) + \sum_p w_p \phi^\dagger_p \phi_p, \quad (2)$$

where $\mathbf{S}$ is a spin-1/2 local moment, the $c_{p\sigma}$'s represent a fermionic band with a constant density of states $\sum_p \delta(\omega - E_p) = N_0$ and on-site spin $\mathbf{s}_c$, and the ϕ_p's represent a bosonic bath having the spectrum in Eq. (1). For fixed $N_0 J_K$, a QCP at $g = g_c$ separates Kondo (or delocalized) and local-moment (or localized) phases. For $g = 0$, the BFKM reduces to the conventional Kondo model.

The partition function associated with $\mathcal{H}_{\text{BFKM}}$ is [8] $Z_{\text{BFKM}} \sim \text{Tr} \exp(-\mathcal{S}'_{\text{imp}})$, where

$$\mathcal{S}'_{\text{imp}} = \int_0^\beta d\tau \left\{ \Gamma S^x(\tau) - \frac{1}{2} \int_0^\beta d\tau' \, S^z(\tau) S^z(\tau') \right.$$
$$\left. \times \left[\chi_0^{-1}(\tau - \tau') - \mathcal{K}_c(\tau - \tau') \right] \right\} \quad (3)$$

and the trace is over the spin degrees of freedom. $\chi_0^{-1}(\tau - \tau')$, with short-time cutoff $\tau_c = 2\pi/\omega_c$, encodes the bath

spectrum. $\mathcal{K}_c(\tau - \tau')$, which has a Fourier transform $\mathcal{K}_c(i\omega_n) = \kappa|\omega_n|$ with $\kappa = \pi N_0 J_K$, comes from integrating out the fermions.

Trotter decomposition of $\mathcal{S}'_{\text{imp}}$ (with time slice τ_0) requires identifying the effect of the transverse-field term ΓS^x with that of a nearest-neighbor term in the corresponding Ising model described [9, 10] by

$$\mathcal{Z} \sim \text{Tr} \exp\left[\sum_{i=1}^{L} K_{\text{nn}} S_i^z S_{i+1}^z + \sum_{i,j=1}^{L} K_{\text{lr}}(i-j) S_i^z S_j^z \right]. \quad (4)$$

The nearest-neighbor interaction $K_{\text{nn}} = -2\ln(\tau_0\Gamma/2)$, while the long-range interaction $K_{\text{lr}}(i-j)$ results from discretizing $\chi_0^{-1}(\tau - \tau') - \mathcal{K}_c(\tau - \tau')$. The bosonic spectrum specified by Eq. (1) gives rise for $\max(\tau_0, \tau_c) \ll \tau < \beta/2$ to a simple power-law behavior along the imaginary-time axis:

$$\chi_0^{-1}(\tau) \sim 1/|\tau|^{2-\epsilon} \qquad \text{for } 0 \leq \epsilon < 1. \quad (5)$$

The inverse temperature $\beta = 1/T$ in the BFKM sets the length $L = \beta/\tau_0$ of the Ising chain, with the periodic boundary condition $S_{L+1}^z = S_1^z$ enforced by the trace operation. Varying the bosonic coupling g amounts to changing the effective temperature $\mathcal{T}$ of the classical model (which bears no relation to T in the BFKM).

Classical Ising chains with this type of long-ranged interaction have been studied for decades, and it is well established that the phase transition for $\epsilon = 0$ is Kosterlitz-Thouless-like [9, 11] and is described over the range $0 < \epsilon < 1$ by a local ϕ^4 theory [3, 12]. For $0 < \epsilon < 1/2$ the phase transition is controlled by the interacting Ginzburg-Wilson-Fisher fixed point, whereas for $1/2 < \epsilon < 1$ mean-field behavior obtains.

In general, if the classical system is below its upper critical dimension, then close to the critical temperature $\mathcal{T}_c$ the only relevant scale is the finite system size, and the static part of the order-parameter correlation function should scale as $\chi_{\text{static}}(L) = L^x Y(L/\xi_\infty)$, where $\xi_\infty \equiv \xi_{\text{static}}(L = \infty) \sim (\mathcal{T} - \mathcal{T}_c)^{-\nu}$. Combined with $\chi_{\text{static}}(L = \infty) \sim (\mathcal{T} - \mathcal{T}_c)^{-\gamma}$, we have $x = \gamma/\nu$. From the hyperscaling relation $\gamma = (2 - \eta)\nu$ and the fact [3] that $\eta = 1 - \epsilon$, we end up with $x = 1 - \epsilon$: at $\mathcal{T} = \mathcal{T}_c$,

$$\chi_{\text{static}}(L) \sim L^{1-\epsilon} \qquad \text{for } 0 < \epsilon < 1/2. \quad (6)$$

Above the upper critical dimension, the finite-size scaling is complicated by the presence of dangerously irrelevant variables that introduce additional scales to the problem and destroy hyperscaling [13]. Extensive theoretical work [13, 14] has concluded that at $\mathcal{T} = \mathcal{T}_c$,

$$\chi_{\text{static}}(L) \sim L^{1/2} \qquad \text{for } 1/2 < \epsilon < 1. \quad (7)$$

Beyond the static limit, the full scaling properties of the susceptibility have not been clarified. We are aware only of a finding (Fig. 4 of [15]) that $\chi(\tau, L)$ fails to show

any scaling collapse in terms of τ/L. Separately, a study of the phase diagram has hinted at the importance of the winding of the interaction around the finite-size Ising ring [16]. These considerations motivate us to carry out a careful analysis of the scaling of χ with particular attention to the effects of winding.

Finite-size scaling of the classical Ising chain.—The interaction $\chi_0^{-1}(\tau - \tau')$ is specified by $\tilde{\chi}_0^{-1}(\omega) \equiv \text{Im}\chi_0^{-1}(\omega + i0^+) = \pi g^2 \omega^{1-\epsilon}\text{sgn}(\omega)$, which follows from Eq. (1) with the cutoff ω_c taken to infinity:

$$\chi_0^{-1}(\tau - \tau') = \int_0^\infty d\omega\, \tilde{\chi}_0^{-1}(\omega) \frac{\cosh\left[\omega(\beta/2 - |\tau - \tau'|)\right]}{\sinh(\omega\beta/2)}$$
$$\equiv \chi_0^{-1}(\tau - \tau', T, \infty), \quad (8)$$

where

$$\chi_0^{-1}(\tau, T, M) = \pi\Gamma(2-\epsilon)g^2 \sum_{n=0}^{M-1} \left[\left(|\tau| + n\beta\right)^{-(2-\epsilon)}\right.$$
$$\left. + \left((n+1)\beta - |\tau|\right)^{-(2-\epsilon)}\right]. \quad (9)$$

We study the Ising chain with effective spin-spin interaction $\chi_0^{-1}(\tau - \tau', T, M)$ for different values of M, the maximum number of times that the interaction wraps around the Ising ring of length L. The $|\tau - \tau'| \to \infty$ behavior is not altered by choosing a finite value of M. We use a cluster-updating Monte Carlo scheme [17, 18] to measure the dynamical susceptibility $\chi(\omega_n, T)$ at coupling $g = g_c$ (i.e., $\mathcal{T} = \mathcal{T}_c$ in the classical model); $\omega_n = 2\pi n/(\tau_0 L)$, $n = 0, \pm 1, \pm 2, \ldots$ are the Matsubara frequencies of the quantum model. A binning analysis of our data shows that the relative error $\Delta\chi/\chi \lesssim 10^{-2}$ and the integrated autocorrelation time is small.

For $0 < \epsilon < 1/2$, the scaling properties do not depend on the choice of M and the static susceptibility obeys Eq. (6). As a result, the dynamic susceptibility scales as

$$\chi(\omega_n, T) = T^{-(1-\epsilon)}\Phi(\omega_n/T). \quad (10)$$

Figure 1 illustrates this ω_n/T scaling for $\epsilon = 0.4$ with $M = 1$ [part (a)] and $M = 10^9$ [part (b)].

For $1/2 < \epsilon < 1$, by contrast, the scaling properties depend crucially on M, as exemplified in Fig. 1 for $\epsilon = 0.8$. The scaling plot for $M = 1$ [part (c)] implies that $\chi(\omega_n) \sim |\omega_n|^{-0.2}$ and $\chi(T) \sim T^{-0.2}$. Only for $M \to \infty$ do we recover the anticipated mean-field result of Eq. (7), as shown in Fig. 1(d) for $M = 10^9$. Between these extremes, there is a slow crossover with increasing M, exemplified by the evolution of $\chi_{\text{static}}(T)$ [19]. Difficulty in recovering mean-field physics in this model has been observed in the context of the phase diagram [16], but the origin of this behavior and its implication for ω_n/T scaling have not previously been recognized.

In obtaining Fig. 1, we set $\kappa = 0$ and $K_{\text{nn}} = 0$ because the construction of clusters via continuous bond probabilities is efficient only for pure power-law interactions
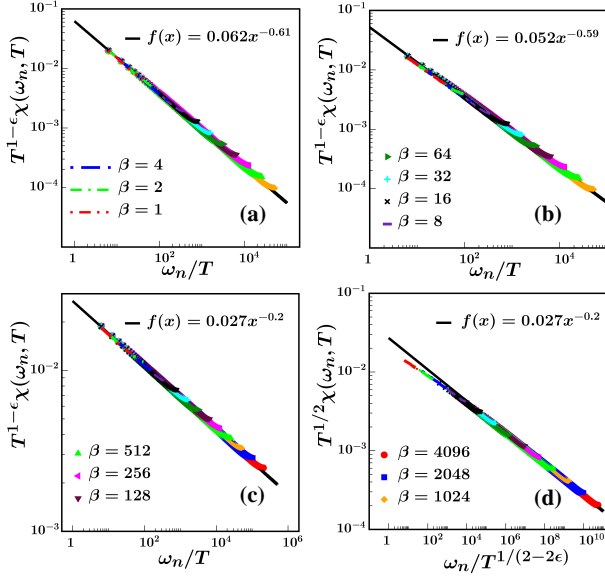
FIG. 1: (Color online) Finite-size scaling of the susceptibility below ($\epsilon = 0.4$, upper panels) and above ($\epsilon = 0.8$, lower panels) the upper critical dimension, for $\tau_0 = 1/16$, $\kappa = K_{nn} = 0$, and winding numbers (a,c) $M = 1$ and (b,d) $M = 10^9$. For $\epsilon > 1/2$, the temperature scaling depends on the choice of M. Similar results have been obtained for various τ_0 between $1/4$ and $1/64$.
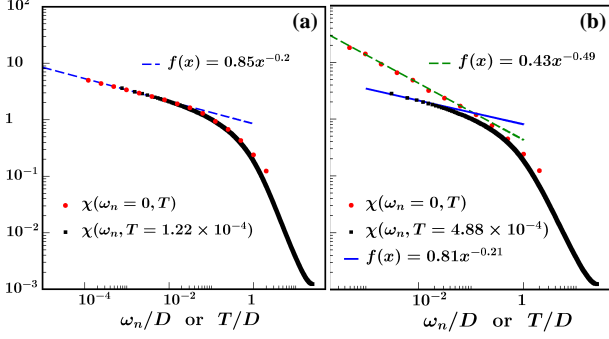

FIG. 2: (Color online) Static and dynamical susceptibilities for $\epsilon = 0.8$ with $\kappa = 2$ and K_{nn} specified by $\Gamma = 0.75$ and $\tau_0 = 1/8$: (a) $M = 1$, and (b) $M = 5 \times 10^7$.

[17]. For nonzero κ and K_{nn}, the calculations can be carried out only for a more limited range of ω_n and T, but the same behavior is found, as illustrated in Fig. 2.

The difference between the cases of infinite and zero winding can be understood as follows. The infinite-winding interaction $\chi_0^{-1}(\omega_n, T, M = \infty)$ depends only on ω_n. The temperature dependence of $\chi(\omega_n, T)$ is then entirely determined by that of the "spin self-energy"

$$\mathcal{M}(\omega_n, T) \equiv \chi_0^{-1}(\omega_n, T) - 1/\chi(\omega_n, T). \qquad (11)$$

The temperature dependence of $\mathcal{M}$ is controlled by the dangerously irrelevant quartic coupling of the local ϕ^4 theory, and is proportional to $T^{1/2}$. On the other hand,
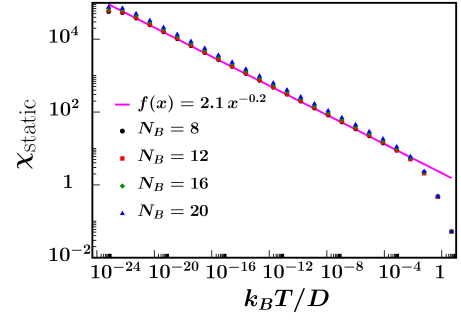

FIG. 3: (Color online) Static susceptibility at the QCP of the Ising BFKM for $\epsilon = 0.8$, calculated using the NRG with discretization $\Lambda = 9$ and various values of the bosonic truncation parameter $8 \leq N_b \leq 20$. See [6] for further details.

the zero-winding interaction $\chi_0^{-1}(\omega_n = 0, T, M = 1) \sim T^{1-\epsilon}$, so $\chi^{-1}(T, \omega_n)$ acquires temperature dependence from both χ_0^{-1} and $\mathcal{M}$. The leading term varies as $T^{1-\epsilon}$, which overpowers the $T^{1/2}$ from the dangerously irrelevant coupling, so the ω/T form of Eq. (10) ensues. We have confirmed that this distinction between $M = 1$ and $M = \infty$ is robust over the range $1/64 \leq \tau_0 \leq 1/4$.

Quantum critical behavior of the BFKM.—We have systematically extended previous NRG calculations [6] to investigate the robustness of the quantum critical behavior. Figure 3 shows data for $\epsilon = 0.8$ that can be fitted to $\chi_{\text{static}}(T) \sim T^{-x}$ over more than 20 decades of T with $x = 1 - \epsilon$ to better than 1% accuracy. The value of the exponent shows no systematic evolution as the bosonic truncation parameter N_B [6] increases from 8 to 20.

These NRG results, which are consistent with ω/T scaling, are in stark contrast with the $\omega/T^{1/(2-2\epsilon)}$ scaling and exponent $x = 1/2$ found in the regime $1/2 < \epsilon < 1$ of the classical Ising chain (with infinite winding). This disparity signals the failure of the quantum-to-classical mapping for the QCP of the Ising BFKM.

The most likely source of the breakdown lies in the replacement of the spin-flip (transverse Kondo-coupling) term in the quantum model by a $(\partial_\tau \phi)^2$ term in the local ϕ^4 theory. In the BFKM, spin flips are essential for the formation of the Kondo-screened state and, by extension, central to the nature of the QCP displaying a critical Kondo effect. (Spin flips are the one-dimensional analog of the vortices in, for instance, the short-range XY model in two dimensions.) In the local ϕ^4 theory, however, the $(\partial_\tau \phi)^2$ term (*i.e.*, the $\omega_n^2 \phi^2$ coupling) is overtaken at low frequencies by the $|\omega_n|^{1-\epsilon} \phi^2$ term associated with the long-range interactions of non-spin-flip type.

To expand on this point, the short-range interaction term in the discrete Ising chain [Eq. (4)] that arises from mapping the transverse Kondo coupling can be expressed

$$\tau_0^2 \log\left(\frac{\Gamma \tau_0}{2}\right) \sum_{i=1}^{L} \frac{(S_{i+1}^z - S_i^z)^2 - \frac{1}{2}}{\tau_0^2}. \qquad (12)$$

In the continuum limit, the corresponding kinetic energy written in terms of $(\partial S^z/\partial \tau)^2$ clearly requires regularization through a finite value of τ_0. The long-range interaction in Eq. (4) must also be regularized, either by reinstating ω_c in $\tilde{\chi}_0^{-1}(\omega)$ entering Eq. (8) or through enforcement of $|\tau - \tau'| > \tau_c$ in Eq. (9). Finally, τ_0 serves to regularize the dynamically generated Kondo scale, $T_K \approx (1/\tau_0)\exp(-1/\Gamma\tau_0)$, below which the quantum scaling occurs. This scale vanishes when τ_0 (or τ_c) vanishes, making the quantum critical behavior inaccessible. These observations suggest that the continuum limit, necessarily taken in the quantum-to-classical mapping, fails to capture the the topological (vortex-like) effect encoded in the Kondo spin-flips. What results is a change in the temperature dependence of the spin self-energy, qualitatively similar to that arising in the classical model from changing the maximum winding from $M = 1$ to $M = \infty$.

A concurrent study [20] addresses the mapping of the dissipative spin-boson model using a Monte Carlo algorithm that explicitly takes the limit $\tau_0 \to 0$ of a classical Ising chain [21]. Ref. [20] focuses on the finite-size scaling exponents of the static magnetic properties, rather than the scaling of the dynamical susceptibility. Its results for the mapped classical action are compatible with, and complementary to, our own. Ref. [20] also speculates that a marginal coupling introduced by bosonic truncation invalidates the NRG results [5] for the spin-boson model. However, our NRG studies for the BFKM, carried out over an extended range of bosonic truncation parameters and covering more than 20 decades of temperature, show evidence, neither for evolution in the exponent x away from its interacting value of $1 - \epsilon$ towards the mean-field $x = \frac{1}{2}$, nor for the line of critical points that would be expected in the presence of a marginal operator. We also note that the NRG conclusion for the BFKM that $x = 1 - \epsilon = y$ cannot be vitiated by a dangerously irrelevant coupling. The NRG result corresponds to a spin self-energy [see Eq. (11)] $\mathcal{M}(T) = \chi_0^{-1} - 1/\chi \sim T^{1-\epsilon}$. In the regime $\frac{1}{2} < \epsilon < 1$ of interest, this temperature dependence dominates any $T^{1/2}$ term potentially generated by a dangerously irrelevant coupling, in a manner reminiscent of what happens in the Monte Carlo calculations with no winding ($M = 1$). These considerations all point to the quantum-to-classical breakdown being a real phenomenon.

In summary, we have addressed the quantum-to-classical mapping of the Ising Bose-Fermi Kondo impurity problem. The finite-size scaling for the spin susceptibility of the mapped classical chain demonstrates an intriguing dependence on the winding of the long-ranged interaction under periodic boundary conditions. Only for infinite winding does one recover the expected mean-field behavior. The contrast between these scaling properties and those of the Bose-Fermi Kondo model suggests a breakdown of the quantum-to-classical mapping for Ising-anisotropic quantum dissipative systems arising from the manner in which Kondo spin flips are treated in the continuum limit that is taken in such a mapping.

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